TITLE: **Mathematically Reduced Chemical Reaction Mechanism Using Neural Networks**

AUTHORS: Butuk, N (PI)

STUDENTS: Garza, A., and Johnson, K

INSTITUTION: Prairie View A & M University
Department of Mathematics
WR Banks Building Room 329
Prairie View, TX 77446-4189

PHONE NO.: 936-857-4021

FAX NO.: 936-857-2019

E-MAIL: n_Butuk@pvamu.edu

GRANT NO.: DE-FG26-03NT-41913

PERIOD OF PERFORMANCE: October, 2003 – September, 2006

DATE: April 11, 2006

1.ABSTRACT

Program Introduction: Rationale and Objectives

The aim of the project is to develop an efficient chemistry model for combustion simulations. The reduced chemistry model will be developed mathematically without the need of having extensive knowledge of the chemistry involved. To aid in the development of the model, Neural Networks (NN) will be used via a new network topology know as Non-linear Principal Components Analysis (NPCA).

Many Combustion systems are modeled by very high-dimensional systems of non-linear differential equations. These equations often exhibit solutions which are un-evenly distributed in phase-space, and which may exist as circles, tori or other manifolds. It is desirable to approximate these isolated regions of the phase-space by a mathematical model of lower dimension than the dimension of the original ambient space. NPCA accomplishes this task using NN.

Accomplishments Achieved During the Current Period of Performance:

The key to this work is a neural network based data reduction method termed Non-linear Principal Components Analysis Neural Networks (NPCA-NN). Given a data set $X \in R^n$, NPCA-NN determines a reduction mapping

$$G: X \rightarrow Y$$

where the set $Y \in R^m$ has reduced dimension $m < n$. Y is then said to be a reduction of X. The inverse mapping reproduces the original data X from the reduced data set Y as

$$H: Y \rightarrow X$$

Hence, NPCA-NN is a composition of mappings which is the same as the identity mapping, i.e.

$$H \text{ o } G: X \rightarrow X$$

The NPCA-NN is a neural network topology with five layers (essentially a combination of two standard Multi-layered Perceptrons), in which the input layer has the same number of nodes as the output layer. This allows the input values to be used as target output values of the network during training. The first part of the network approximates the mapping G. It contains the mapping layer. The middle layer is the bottleneck layer consisting of the m nodes (i.e. desired reduced dimension m). The last part of the network implements the mapping H and contains the de-mapping layer. This layer takes the output of the middle layer and maps it onto the output layer. It is on the bottleneck layer, that the reduced manifold of the chemistry is constructed.

We have developed a training procedure for NPCA-NN that significantly improves it's rate of convergence. The theoretical justification for the approach is sound. The basic idea is as follows. An input signal is fed into several simple networks of much reduced accuracy; which actually are separate parts of one large network. These parts are subsequently trained with a target signal in such a way that the sum of all the outputs approaches the target signal. The first step is to train the first network until saturation of the learning error. Next, leave the first network and train the second network to correct the difference between the target and the output of the first network. We successively add more networks, ideally reducing the error made by the total network by one order of magnitudes; per network. Finally, we connect the trained parts to form a single parallel large network. The combined larger network adds up all previous outputs to given an approximation of the target output.

The last objective of this work is to couple NPCA-NN to a CFD code. Our approach is to couple the NPCA-NN to a simple 2-dimensional Euler solver prior to coupling to a production grade CFD code. Modification of the Euler solver to include chemical reactions is currently under way.

Plans for the Remaining Period of Performance

The remaining tasks in this project include**:**

- Develop the NPCA model on real chemical reaction mechanism data
- Couple NPCA model to a CFD code.

2. LIST OF PUBLICATIONS AND STUDENTS SUPPORTED

Publications

- Non during this period

Students Supported

- Ken Johnson, graduate student expected graduation May, 2006
- Alejandrina Garza, graduate student expected graduation December, 2006